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14. ABSTRACT
The ratio of computational to physical particles is a key factor in determining the statistical scatter and accuracy in particle-based simulation. This is particularly true for problems characterized by wide ranges of number density such as those found in spacecraft electric propulsion plumes as well as ionizing discharges, where populations of electrons and excited states can grow exponentially. A particle management method must then be devised which balances statistical accuracy requirements with prevention of runaway computational costs. The standard approach of splitting and merging of particles [1], however, cannot guarantee simultaneous conservation of mass, momentum and energy using pair-wise coalescence (2:1 ratio), due to the insufficient degrees of freedom. As a result, various sophisticated models have been designed to minimize or internally store the error resulting from these merges (e.g. [2,3]). Some of these involve the interpolation of particle weights onto a grid, a procedure which can be costly and which may introduce diffusion. Instead, we have devised a simpler method [4] which relies on the generation of two particles, providing the required freedom to conserve all moments up to 2nd order exactly. Thus, pair-wise reduction is obtained through an equivalent ratio of 4:2, but particle merges of arbitrary ratios (n+2):2 can be obtained with similar conservation properties. Furthermore, the method can be seen to conserve electrostatic energy using the additional available particle position degrees of freedom. The present work extends this exact moment-preserving merge through an octree-based adaptive mesh in velocity space to ensure that merging partners are relatively close in phase space. This mitigates artificial thermalization due to merging of particles with large opposite velocities such as those found in beam-beam interactions. An analogous particle split method is also described for re-populating depleted- VDFs that result from the particle merging. The combined fully-adaptive particle weighting scheme is then applied to several test-problems, e.g. collisionless thermal beams in a potential well, gas breakdown problem by an ionizing beam, etc., which are designed to characterize and test the limits of the method. Results are also compared to fixed particle weight and simple random 4:2 merging solutions. Extension of the method to higher-order moment conservation is also considered.

15. SUBJECT TERMS

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Moment Preserving Adaptive Particle Weighting Scheme for PIC Simulations

Jean-Luc Cambier & Robert Martin

Spacecraft Propulsion Branch
Air Force Research Laboratory
Edwards Air Force Base, CA USA

39th IEEE International Conference on Plasma Science

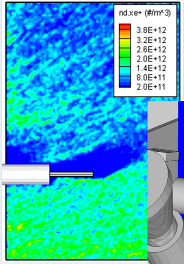
Outline

Spacecraft Plasmas

Spacecraft Propulsion Relevant Plasmas:

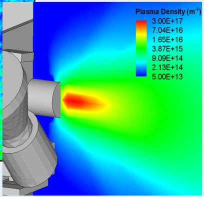
- Plumes from hall thrusters
- Discharge and Breakdown in FRC
- Relevant Densities can Span 6+ Orders of Magnitude
- Good Statistics in Plume Requires Computationally Prohibitive Particle Numbers in Engine
- Tiny Early e^- Populations Critical to Ionization Induction Delay

Electric Propulsion Plumes

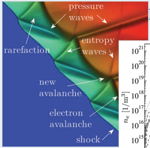


Brieda et. al., AIAA-2006-5023

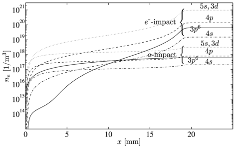
Fife et. al., IEPC-2003



Ionization Breakdown



Kapper & Cambier, J. Appl. Phys. 109, (2011)



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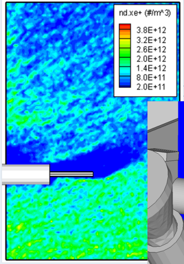
Solution?

Adaptive Physical:Computational Weights

Electric Propulsion Plumes



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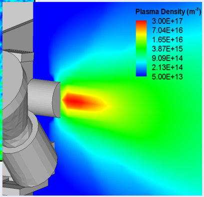

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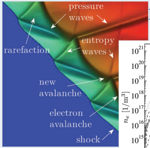

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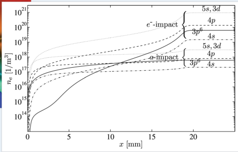

Prior Merging Techniques

Numerous Previous Merge Methods:

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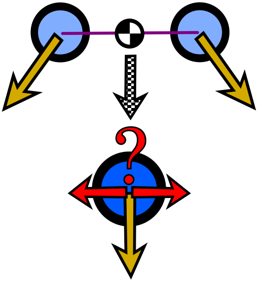
- 2:1 - Cannot Conserve Energy
  (Lapenta & Brackbill, JCP 1994)



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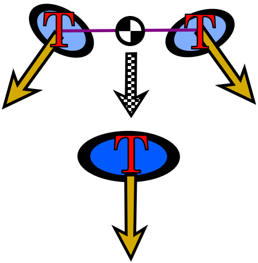

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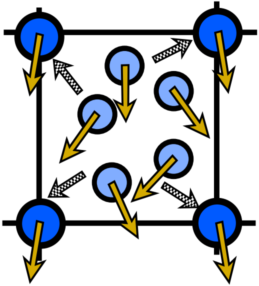

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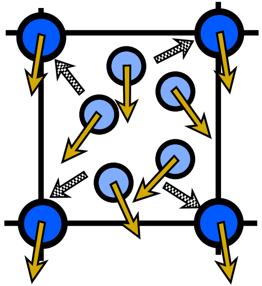
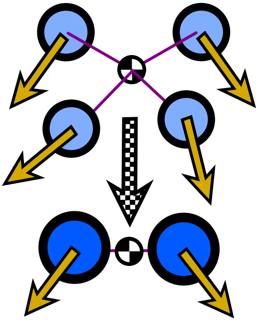
All Introduce Significant Error and/or Complexity



Merge to Pair $\rightarrow$ DOF for Conservation:

- (n+2):2 yields Exact Mass, Momentum, and Kinetic Energy Conservation
- Applied Spatially also Shown to Conserve Electrostatic Energy
- Though Energy Conserving, Still Thermalizes VDF

(Cambier, AFOSR Review 2006)



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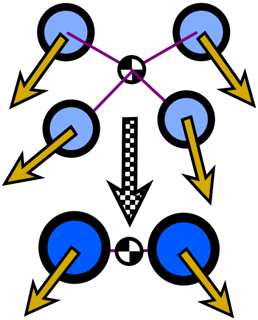
Selection of Near Neighbors in VDF Limits Thermalization

(Like Near Neighbor Selection in Advanced 2:1 Merges to Limit Numerical Cooling)



Advantages of Octree Sort:

- Octree Prevents Merge Across Distribution
- Limits Thermalization
- Conserves Entropy up to Octree Quadrature

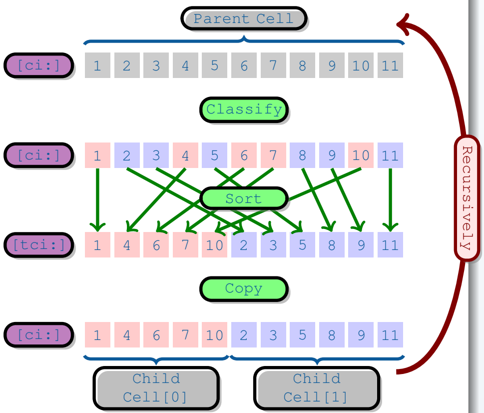
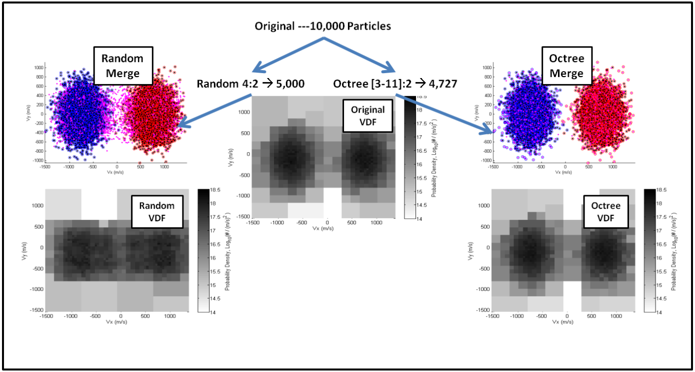


FIGURE: Cell Index Particle Sorting Procedure

Comparison of Random vs. Octree Merge Partner Selection (Note: Mass, Momentum, and Kinetic Energy Both Exactly Conserved)



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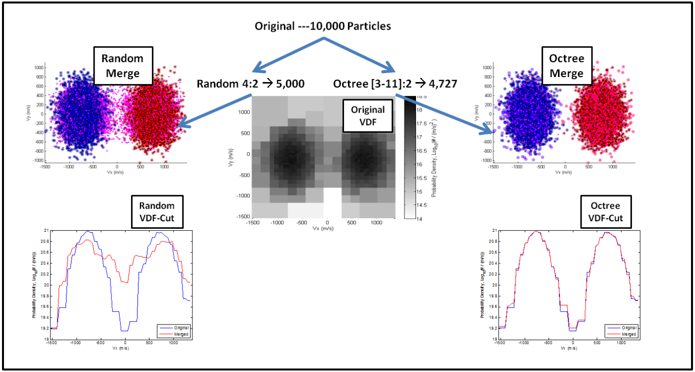
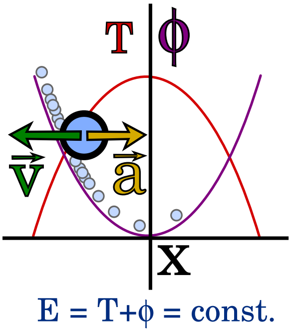


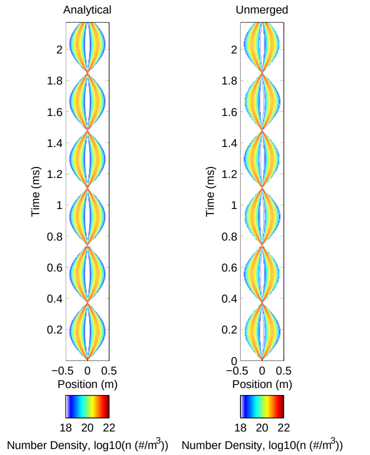
Beam in Potential Well

Collisionless Crossing Beams:

- Particles in Parabolic Potential Well
- Constant Potential
- Collisionless -> Known Trajectory, $x(t)$
- Sinusoidal Path from Initial Velocity
- Analytical Solution for Density, $n(x, t)$
- Crank-Nicolson Particle Simulations
- C-N is Stable and Non-Dissipative for Re(λ)=0



- 6000 Unmerged Particles
- Reproduces 3-4 Orders of Magnitude



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- Random Merge -> Thermalization
- 3000 First Point, 1500 First Cross
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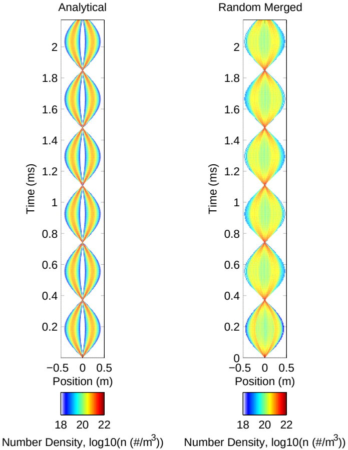

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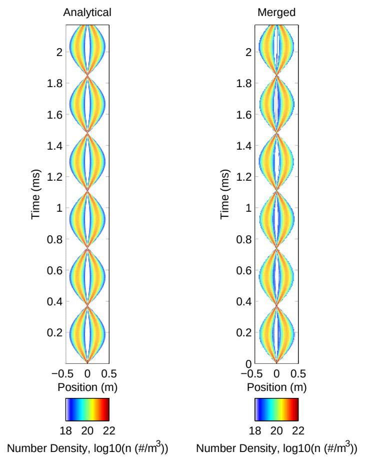

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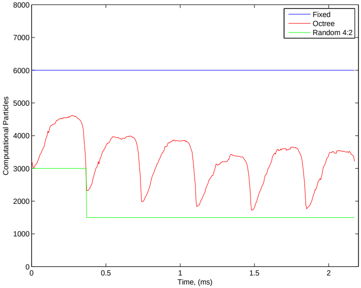

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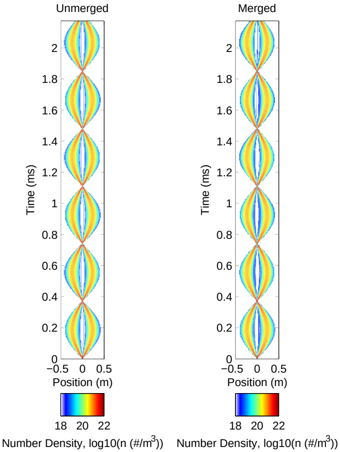
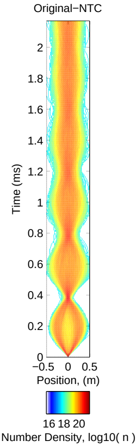
- Merge & Split Adapts Particle Count
- Despite Continuous Weight Scaling, Similar Results over Several Bounces



- Initial Bi-Maxwellian Distribution in Potential Well

COLLISIONAL BEAMS IN POTENTIAL WELL

- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization



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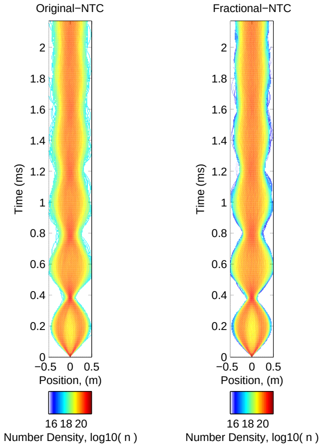

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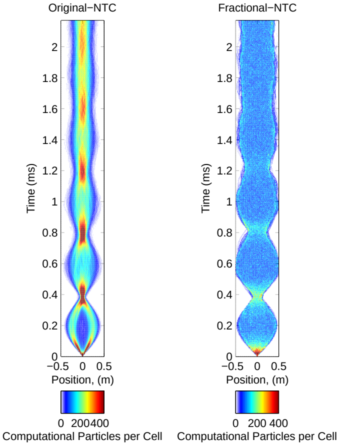
- Particles/Cell Dramatically Different



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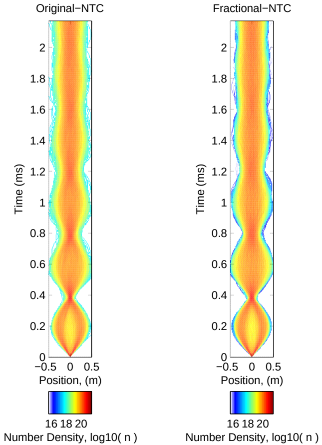
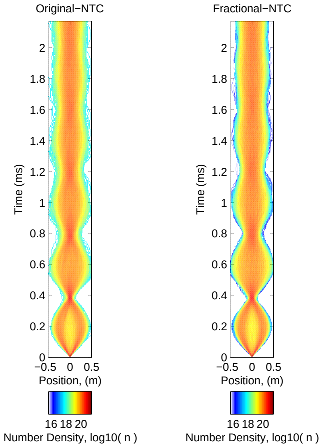


Collisional Beams in Potential Well

- Initial Bi-Maxwellian Distribution in Potential Well
- NTC Collisions Results in Beam Thermalization
- Fractional-NTC Collisions Produce Same Behavior
- Particles/Cell Dramatically Different
- Fringe Extends to Lower Densities with Variable Weights
- Relative ‘Error’ Unknown without Analytical Solution or High Fidelity Simulation



Gas Breakdown

- Merge Needed w/ Exponential # Growth

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- Examples...
  Chain Branching: $H_2 + M \rightarrow 2H + M$
  Ionization: $Ar^0 + e^- \rightarrow Ar^+ + e^- + e^-$

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  Chain Branching: $H_2 + M \rightarrow 2H + M$
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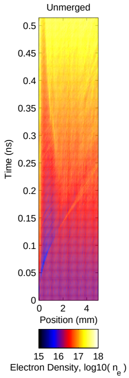
- Ionizing Breakdown in 6kV Potential
- Electrons Flow from Cathode $\rightarrow$ Anode
- Inelastic MCC with Background
- Potential Function of e^- and Ar^+



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  Chain Branching: $\mathrm{H_2} + \mathrm{M} \rightarrow 2\mathrm{H} + \mathrm{M}$
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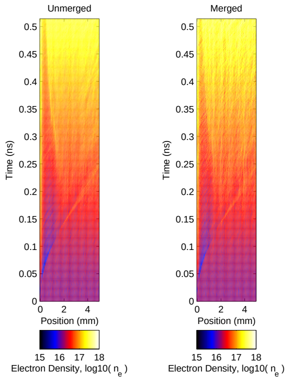
- Potential Function of e^- and Ar^+
- Merge Retains Features and Magnitude



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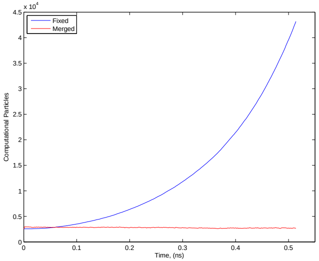
While Controlling Computational Cost



- Moments defined as Integrals of VDF: $\overline{Q} = \int Qnfdv_i$
- Discrete Version: $nf \to w^{(p)}\delta(v^{(p)})$ such that $\overline{Q} = \sum w^{(p)}Q / \sum w^{(p)}$
- Merged Particles have 4 DOF each: w, v_x, v_y, v_z
- Number of Moments Conserved from Number of DOF

Moment	Order	

Cartesian Moments

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Moment	Order	
Mass	0^{th}	$\sum w^{(p)} = \overline{w}$
Mass Flux	1^{st}	$\sum w^{(p)} v_i^{(p)} = \overline{w} \cdot \overline{v_i}$

1 Particle - Mass & Momentum

Cartesian Moments

$\overline{w}$ & $\begin{bmatrix} \overline{v_x} \\ \overline{v_y} \\ \overline{v_z} \end{bmatrix}$

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Momentum Flux	2^{nd}	$\sum w^{(p)} v_i^{(p)} v_i^{(p)} = \overline{w} \cdot \overline{v_i v_i}$

2 Particles - Mass, Momentum, and Diagonal 2^{nd}: $\overline{\overline{P}}$

Cartesian Moments

$$\begin{bmatrix} \overline{v_x v_x} & \overline{v_x v_y} & \overline{v_x v_z} \\ \overline{v_x v_y} & \overline{v_y v_y} & \overline{v_y v_z} \\ \overline{v_x v_z} & \overline{v_y v_z} & \overline{v_z v_z} \end{bmatrix}$$

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3 Particles - Mass, Momentum, Full 2^{nd}: $\overline{\overline{P}}$ & τ_{ij}

Cartesian Moments

$$\begin{bmatrix} \overline{v_x v_x} & \overline{v_x v_y} & \overline{v_x v_z} \\ \overline{v_x v_y} & \overline{v_y v_y} & \overline{v_y v_z} \\ \overline{v_x v_z} & \overline{v_y v_z} & \overline{v_z v_z} \end{bmatrix}$$

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Momentum Flux	2^{nd}	$\sum w^{(p)} v_i^{(p)} v_j^{(p)} = \overline{w} \cdot \overline{v_i v_j}$
Energy Flux	3^{rd}	$\sum w^{(p)} v_i^{(p)} (v^{(p)})^2 = \overline{w} \cdot \overline{v_i v^2}$

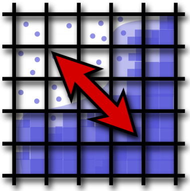
4 Particles - Mass, Momentum, Full 2^{nd}, Energy Flux: q_i

Cartesian Moments

$$\begin{bmatrix} \overline{v^2 v_x} \\ \overline{v^2 v_y} \\ \overline{v^2 v_z} \end{bmatrix}$$

Merge Quantities Needed for Hybridization:

- Reconstructed VDF Natural extension to Fokker-Planck/Boltzmann Solvers
- Higher Moment Merges would Facilitate extension to Hybrid Euler, Navier-Stokes, 13-moment, and Beyond
- Reversal of VDF/Moments to Particles would Enable Particle Generation in Transition Zones



Thank You

Questions?